

Effect of surface roughness and adsorbates on superlubricity

V.N. Samoilov,^{1,2} C. Yang,¹ U. Tartaglino,^{1,3} and B.N.J. Persson¹

¹IFF, FZ-Jülich, 52425 Jülich, Germany

²Physics Faculty, Moscow State University, 117234 Moscow, Russia

³Democritos National Simulation Center, Via Beirut 2, 34014 Trieste, Italy

We study the sliding of elastic solids in adhesive contact with flat and rough interfaces. We consider the dependence of the sliding friction on the elastic modulus of the solids. For elastically hard solids with planar surfaces with incommensurate surface structures we observe extremely low friction (superlubricity), which very abruptly increases as the elastic modulus decreases. We show that even a relatively small surface roughness or a low concentration of adsorbates may completely kill the superlubricity state.

This manuscript has been published in the book: “Superlubricity”, edited by A. Erdemir and J.-M. Martin, Elsevier, Amsterdam (2007). The copyright of the final version of this paper has been transferred to Elsevier.

1. Introduction

Friction between solid surfaces is a very important phenomenon for biology and technology [1] and it is very common in nature. Static friction always involves the coexistence of different metastable configurations at microscopic level. When one surface slides on the other at low speed, first there is a loading phase during which the actual configuration stores elastic energy. Then, when the stored energy is large enough, an instability arises [2, 3, 4]: the system jumps abruptly to another configuration and releases elastic energy into irregular heat motion. The exact way of how the energy is dissipated does not influence the sliding friction force, provided that the dissipation is fast enough to happen before the next sliding event.

There are many possible origins of elastic instabilities, e.g., they may involve individual molecules or, more likely, groups of molecules or “patches” at the interface, which have been named stress domains [5, 6, 7, 8]. As a result the overall motion may not exhibit any stick and slip behavior at macroscopic level, since the local rearrangements can occur at different times in an incoherent manner. Moreover, at least at zero temperature, the friction force does not vanish in the limit of sliding speed $v \rightarrow 0$, but it tends to some finite value which depends on the average energy stored during the loading events.

On the other hand, a system without instabilities cannot present a non-vanishing kinetic friction as $v \rightarrow 0$: if for any sliding distance there exist only one stable configuration, the energy stored at the interface is a single-valued function of the relative sliding distance. Thus when sliding occurs slowly the process has to be reversible, i.e., with negligible friction.

If the structure of the two contacting surfaces do not match, the formation of pinned states is hindered: when some groups of atoms are in registry with the other surface, occupying a local energy minimum, some other groups of atoms cannot adjust to the local energy-minimum configuration without a deformation of the

solids. In this case there is a competition between two energies: the lateral corrugation of the interaction potential between the walls, and the elastic energy to deform the solid so that every surface patch adjusts into a local minimum. If the latter prevails, the system is pinned and static friction appears. Otherwise, if the solid is sufficiently stiff, local domains do not show any instability and can overcome reversibly the local barriers. The overall effect is a motion with no static friction, since when some domains move uphill some other regions move downhill, so that the total energy is constant. This absence of instabilities due to a mismatch of the two surfaces’ structures has been named *superlubricity* [9], although a more appropriate name would have been *structural lubricity* [10].

It is well known that elastically hard solids tend to exhibit smaller sliding friction than (elastically) soft materials [11]. One extreme example is diamond which under normal circumstances exhibits very low kinetic friction coefficient, of the order of 0.01, when diamond is sliding on diamond. This can be explained by the nearly absence of elastic instabilities because of the elastic hardness of the material.

Recently, superlubricity has been observed during sliding of graphite on graphite: in the experiment described in Ref. [12] a tungsten tip with a graphite flake attached to it is slid on an atomically flat graphite surface. When the flake is in registry with the substrate stick-slip motion and large friction are observed. When the flake is rotated out of registry, the forces felt by the different atoms start to cancel each other out, causing the friction force to nearly vanish, and the contact to become superlubric.

Graphite and many other layered materials are excellent dry lubricants. The most likely reason for this is that the solid walls of the sliding objects get coated by graphite flakes or layers with different orientation so a large fraction of the graphite-graphite contacts will be in the superlubric state. This will lead to a strong reduction in the average friction. However, the coated solid

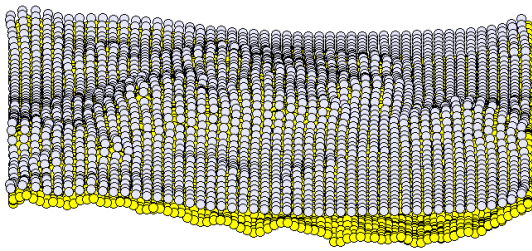


FIG. 1: The contact between an elastic block with a flat surface and a rough *rigid* substrate. Only the interfacial layers of atoms are shown. The elastic modulus of the block is $E = 100$ GPa. The substrate is self-affine fractal with the root-mean-square roughness 3 Å, fractal dimension $D_f = 2.2$. The applied pressure $p = 10$ GPa.

walls are unlikely to be perfectly flat and clean, and it is important to address how surface roughness and adsorbates may influence the superlubric state. Here we will show that even a relatively small surface roughness or low adsorbate coverage may kill the superlubric state.

2. Model

The results presented below have been obtained for an elastic flat block sliding on a rigid substrate. We considered both flat and rough substrates. The atoms in the bottom layer of the block form a simple square lattice with lattice constant a . The lateral dimensions $L_x = N_x a$ and $L_y = N_y a$. For the block, $N_x = N_y = 48$. Periodic boundary conditions are applied in the xy plane. We have used a recently developed multiscale molecular dynamics model, where the block extends in the vertical z -direction a similar distance as along the x -direction [13] (see also [14]).

The lateral size of the block is equal to that of the substrate, but for the latter we use a different lattice constant $b \approx a/\phi$, where $\phi = (1 + \sqrt{5})/2$ is the golden mean, in order to hinder the formation of commensurate structures at the interface. For the substrate, $N_x = N_y = 78$. The mass of a block atom is 197 a.m.u. and the lattice spacing of the block is $a = 2.6$ Å, so to get the same atomic mass and density of gold. The lattice spacing of the substrate is $b = 1.6$ Å. We consider solid blocks with different Young's moduli from $E = 0.2$ GPa up to 1000 GPa. The Poisson ratio of the block is $\nu = 0.3$.

Many surfaces tend to be nearly self-affine fractal. A self-affine fractal surface has the property that if part of the surface is magnified, with a magnification which in general is appropriately different in the perpendicular direction to the surface as compared to the lateral directions, then the surface “looks the same”, i.e., the statistical properties of the surface are invariant under this scale transformation [13, 15]. For a self-affine sur-

face the power spectrum has the power-law behavior

$$C(q) \sim q^{-2(H+1)}, \quad (1)$$

where the Hurst exponent H is related to the fractal dimension D_f of the surface via $H = 3 - D_f$. Of course, for real surfaces this relation only holds in some finite wave vector region $q_0 < q < q_1$, and in a typical case $C(q)$ has a roll-off wavevector q_0 below which $C(q)$ is approximately constant.

In our calculations we have used self-affine fractal surfaces generated as outlined in Ref. [15], with the fractal dimension $D_f = 2.2$ and the roll-off wavevector $q_0 = 3q_L$, where $q_L = 2\pi/L_x$. We have chosen $q_0 = 3q_L$ rather than $q_0 = q_L$ since the former value gives some self-averaging and less noisy numerical results. We also used $q_1 = 2\pi/b = 78q_0$.

The atoms at the interface between the block and the substrate interact with the Lennard-Jones potential

$$U(r) = 4\epsilon \left[\left(\frac{r_0}{r} \right)^{12} - \left(\frac{r_0}{r} \right)^6 \right], \quad (2)$$

where r is the distance between a pair of atoms. In the calculations presented below we have used $r_0 = 3.28$ Å and $\epsilon = 40$ meV, which gives an interfacial binding energy (per unit area) $\Delta\gamma \approx 4\epsilon/a^2 \approx 24$ meV/Å².

As an illustration, in Fig. 1 we show the contact between a flat elastic block (top) and a randomly rough *rigid* substrate (bottom). Only the interfacial block and substrate atoms are shown. Note the elastic deformation of the block, and that non-contact regions occur in the “deep” valleys of the substrate.

In all results presented below the upper surface of the block moves with the velocity $v = 0.1$ m/s, and the (nominal) squeezing pressure p , if not stated otherwise, is one tenth of the elastic modulus E of the block, i.e., $p = 0.1E$. We did also some test calculations for $v = 1$ m/s (not shown) but found very similar results as for $v = 0.1$ m/s. In fact, neglecting heating effects, one does not expect any strong dependence of the friction force on the velocity, as long as it is much smaller than the sound velocity (typically 1000 m/s), and much higher than the velocities where thermally activated creep motion becomes important (usually a few μ m/s). Furthermore, the sliding direction does not play a significant role since the commensurability ratio $8/13$ is the same along the x and y directions. For the (randomly) rough surfaces we did some test calculations where we reversed the sliding direction and found that the friction force changed by at most 20%. This is a finite-size effect: for an infinite system sliding along the positive or negative x -axis cannot change the friction force.

The reason for choosing p proportional to E is twofold. First, we consider solids with elastic modulus which varies over several orders of magnitude, and it is not possible to use a constant p as this would result in unphysical large variations in the elastic deformation of the

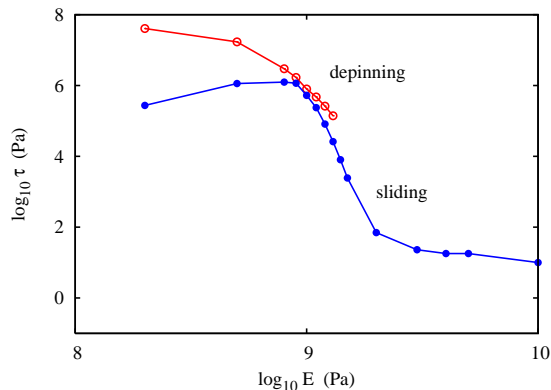


FIG. 2: The shear stress at depinning (static friction) and during sliding (kinetic friction) as a function of the elastic modulus E of the block, for the flat substrate. In the calculation we have used the squeezing pressure $p = 0.1E$ and the sliding velocity $v = 0.1$ m/s.

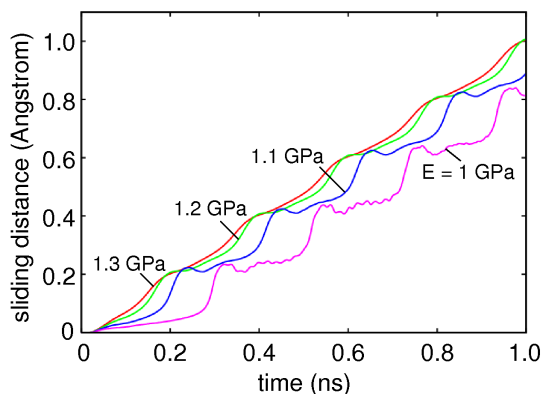


FIG. 3: The average displacement of the interface block atoms (in the sliding direction) as a function of time, for the flat substrate. The elastic modulus of the block is $E = 1, 1.1, 1.2$ and 1.3 GPa. The transition from high friction (stick-slip) to superlubricity (steady sliding) is demonstrated clearly.

block. Second, if two elastic solids are squeezed together with a given load, then as long as the area of real contact is small compared to the nominal contact area, the pressure in the contact areas will be proportional to the elastic modulus of the solids [16].

The system is kept at low temperature by a viscous friction (a Langevin thermostat at $T = 0$ K) applied only to the topmost layers of block atoms, which are far away from the interface. On the time-scale of our simulations we observed no significant variation in the frictional shear force which could be attributed to a (slow) heating up of the system.

3. Numerical results

We first consider the sliding of clean smooth and rough surfaces for elastic solids with different elastic modulus

and surface roughness. We also study the influence of adsorbed molecules on sliding friction. We show that already a small surface roughness or less than a monolayer of adsorbed molecules may strongly increase the friction.

3.1. Clean smooth and rough surfaces

Let us first assume that both the block and the substrate have atomically smooth surfaces. Fig. 2 shows the shear stress as a function of the elastic modulus E of the block. Note the relatively abrupt decrease in the friction when the elastic modulus changes from $E_1 \approx 0.7$ GPa to $E_2 \approx 2$ GPa. For $E > E_2$ practically no instabilities occur and the friction is extremely small, while for $E < E_1$ relatively strong elastic instabilities occur at the sliding interface, and the friction is high. For $E = 0.2$ GPa the static friction $\mu_s > 2$. This calculation illustrates that the transition from high friction to *superlubricity* can be very abrupt; in the present case an increase in the elastic modulus by only a factor of 3 (from 0.7 to 2.1 GPa) decreases the kinetic friction by a factor of $\sim 10^5$.

We have studied the variation of the shear stress as a function of time when the elastic modulus of the block equals (a) $E = 0.8$ GPa and (b) $E = 2$ GPa. When the elastic modulus of the solid is above the superlubricity threshold as in case (b), no significant elastic instabilities occur; the stress is a periodic function of time, with the period corresponding to the displacement 0.2 Å. For softer solids, when strong elastic instabilities occur during sliding as in case (a), the shear stress is less regular (and the arrangement of the interfacial block atoms more disordered) than for the stiffer solid, and the (average) period is *longer* than 0.2 Å.

The remarkable abruptness of the superlubricity transition is illustrated in Fig. 3, which shows the average displacement of the interface block atoms (in the sliding direction) as a function of time, for the flat substrate. Note the onset of stick-slip as the elastic modulus of the block decreases from $E = 1.3$ GPa (upper curve) to 1 GPa (lower curve).

The regular pattern with period 0.2 Å has a simple geometrical explanation related to the commensurability ratio $8/13$ along the sliding direction: in the ground state each block's atom has 8 allowed positions within the cell b of the substrate. Hence there are 8 equivalent configurations within a sliding distance $b = 1.6$ Å.

Let us now consider the influence of surface roughness on the sliding dynamics. In Fig. 4 we show the average shear stress for an elastic block sliding on a rough substrate, as a function of the elastic modulus E of the block. For the substrate with the largest roughness, no superlubricity state can be observed for any elastic modulus up to $E = 10^{12}$ Pa.

Our results are in agreement with the theoretical predictions of Sokoloff [17]: roughness on multiple length scales can induce a transition from a *weak pinning regime*

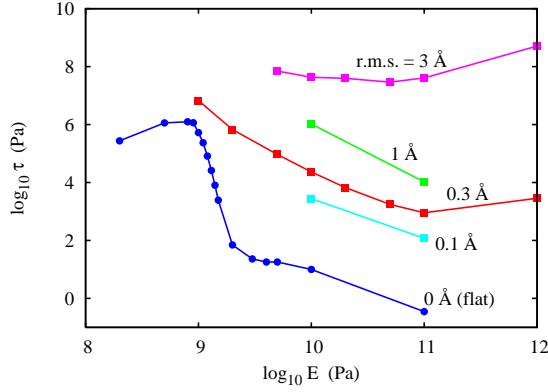


FIG. 4: The shear stress for an elastic block sliding on rough substrates, as a function of the elastic modulus E of the block. The curves from top to bottom correspond to the root-mean-square roughness amplitudes of the fractal substrate 3, 1, 0.3, 0.1 Å and 0 Å (flat substrate).

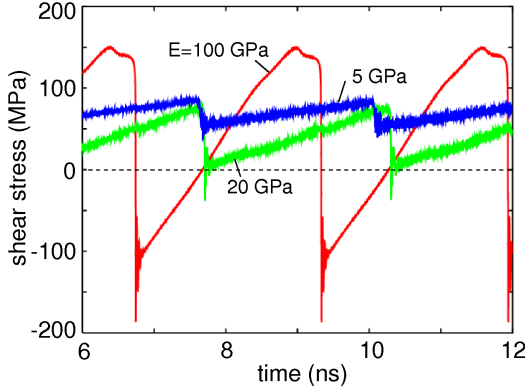


FIG. 5: The shear stress as a function of time for the rough substrate with the root-mean-square roughness amplitude 3 Å. The elastic modulus of the block is $E = 100$, 20 and 5 GPa.

to a *strong pinning regime*. The main difference between our model and the one of Sokoloff is that the latter assumes purely repulsive interactions between the atoms, while here the attractive part of the Lennard-Jones potential gives rise to an adhesive pressure p_{ad} which will contribute to the effective load. Since in our case $p_{ad} \approx 10$ GPa, the shear stress that we obtain is almost independent of the external load.

We have also studied the shear stress as a function of time for different elastic moduli, see Fig. 5. Note that in addition to major slip events, several small slip events occur in all cases. These events correspond to local slip at some asperity contact regions before the major slip involving the whole contact area. In all cases, the time dependence of the shear stress remains periodic with the period 2.6 Å, which corresponds to the lattice spacing of the block. At the current sliding speed $v = 0.1$ m/s the kinetic friction force is smaller for the stiffer solid

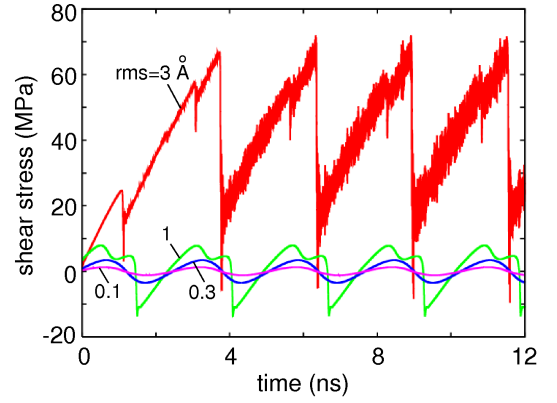


FIG. 6: The shear stress as a function of time for the rough substrate with the root-mean-square roughness amplitudes 3, 1, 0.3 and 0.1 Å. The elastic modulus of the block is $E = 10$ GPa. The transition from high friction to superlubricity is clearly demonstrated.

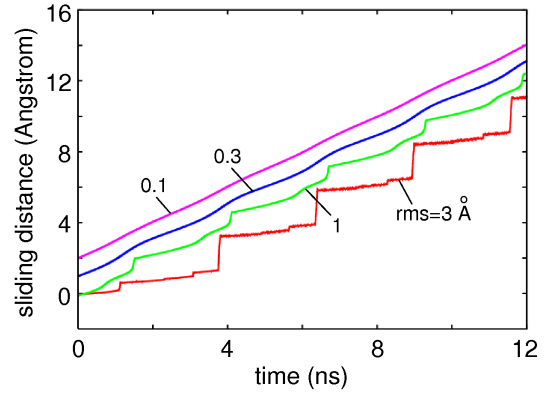


FIG. 7: The average displacement of the interface block atoms (in the sliding direction) as a function of time for the rough substrate with the root-mean-square roughness amplitudes 3, 1, 0.3 and 0.1 Å. The elastic modulus of the block is $E = 10$ GPa. The transition from high friction (stick-slip) to superlubricity (steady sliding) is clearly demonstrated.

even if the load is larger: although the maximum shear stress achieved before sliding is quite big in such case, the average shear stress is small and part of the elastic energy stored in the loading phase is not dissipated, but it is given back to the system. For the elastically softer blocks ($E = 20$ and 5 GPa), the stress-noise increases after each major slip event; this is caused by the elastic waves (heat motion) excited during the (major) rapid slip events and not completely adsorbed by the thermostat.

In Fig. 6 we show the effect of the substrate root-mean-square (rms) roughness amplitude on the shear stress as a function of time for the block with the elastic modulus $E = 10$ GPa. We varied the root-mean-square roughness amplitude from 3 to 0.1 Å. For the rms roughness amplitudes 0.3 and 0.1 Å the major slip is not as abrupt as for higher roughness amplitudes. In all cases, the time

dependence of the shear stress remains periodic with the period 2.6 \AA determined by the lattice spacing of the block. For the rms roughness 3 \AA two small and a major slip events can be observed in each period, and the kinetic friction is high. For the case with the rms amplitudes 0.3 and 0.1 \AA (almost) no elastic instability occurs, and the kinetic friction is very small.

In Fig. 7 we show the average displacement of the interface block atoms (in the sliding direction) as a function of time for the block with the elastic modulus $E = 10 \text{ GPa}$, and for the rough substrate with various roughness amplitudes. The transition from high (stick-slip) friction for the most rough surface to very low friction (smooth sliding) for the surfaces with root-mean-square roughness 0.3 and 0.1 \AA is demonstrated clearly.

3.2. Dependence of the friction on the load

We now study the dependence of the friction force on the load. We consider both flat surfaces and the case where the substrate is rough. For flat surfaces the frictional shear stress is independent of the squeezing pressure p as long as p is smaller than the adhesion pressure p_{ad} which is of the order of 10^{10} Pa . For rough surfaces the situation is more complex and the frictional shear stress will depend on the squeezing pressure p even for very small p unless at least one of the solids is so compliant that the attractive interaction becomes important for the contact mechanics.

Flat surface

During sliding, the atoms at the sliding interface will experience energetic barriers derived from both the attractive interaction between the atoms on the two opposing surfaces, and from the applied load. Thus, we may define an *adhesion pressure* p_{ad} , and as long as $p_{\text{ad}} \gg p$, where p is the pressure in the contact area derived from the external load, the frictional shear stress will be nearly independent of the applied load. Let us first consider the limiting case where the elastic modulus of the block is extremely small. In this case, in the initial pinned state (before sliding) all the block atoms will occupy hollow sites on the substrate, as indicated by atom **A** in Fig. 8. During sliding along the x -direction, the atom **A** will move over the bridge position **B** and then “fall down” into the hollow position **C** (we assume overdamped motion). The minimum energy for this process is given by the barrier height $\delta\epsilon$ (the energy difference between the sites **B** and **A**) plus the work $pa^2\delta h$ against the external load, where a is the block lattice constant and δh the change in the height between sites **B** and **A** (which depends on p). Thus the frictional shear stress σ_f is determined by $\sigma_f a^2 b = \delta\epsilon + pa^2\delta h$, or

$$\sigma_f = \delta\epsilon/(ba^2) + p\delta h/b = (p_{\text{ad}} + p)\delta h/b,$$

where we have defined the adhesion pressure $p_{\text{ad}} =$

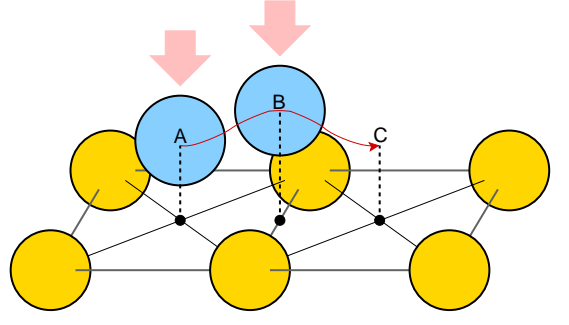


FIG. 8: A block atom moving (or jumping) from the hollow site **A** over the bridge site **B** to the hollow site **C**. The maximum energy position along the trajectory is at site **B**.

$$\delta\epsilon/(a^2\delta h).$$

In our case $\delta\epsilon \approx 3 \text{ meV}$ and $\delta h \approx 0.008 \text{ \AA}$ giving $p_{\text{ad}} \approx 10^{10} \text{ Pa}$. Thus, in the present case, only when the local pressure in the contact regions becomes of the order of $\sim 10 \text{ GPa}$, or more, it will start to influence the shear stress. This result is in accordance with our simulation results. Thus, for smooth surfaces, the shear stress acting on the block with the elastic modulus $E = 0.5 \text{ GPa}$, squeezed against the substrate with the pressure $p = 50$ and 150 MPa , is identical ($\approx 1 \text{ MPa}$) within the accuracy of the simulations.

Rough surface

In the absence of adhesion, contact mechanics theories predict that the area of real contact A between two elastic solids with randomly rough (but nominally flat) surfaces is proportional to the squeezing force (or load) F_N as long as $A \ll A_0$ (where A_0 is the nominal contact area). The law $A = \alpha F_N$ holds strictly only if the roughness occurs on many different length scales [18], but this is (almost) always the case for natural surfaces (e.g., a stone surface) or surfaces of engineering interest. For an infinite system (thermodynamic limit) not only A is proportional to F_N , but the distribution of sizes of the contact regions, and the stress distribution in the area of real contact, is independent of the squeezing force if $A \ll A_0$. The physical picture behind these results is that as the squeezing force increases, new contact regions are formed in such a way that the quantities referred to above remain unchanged. However, for any finite sized system this picture cannot hold exactly as it requires that some contact regions have infinite-size, which is possible only for an infinite sized system.

When the attractive interaction cannot be neglected, the area of real contact is often assumed [19] to be of the form $A \approx \alpha(F_N + F_{\text{ad}})$ where F_{ad} represents an adhesive load, but this relation is only approximate [18, 20]. If the friction force F_f is assumed to be proportional to the area of real contact, then one expects $F_f = \sigma_c A \approx$

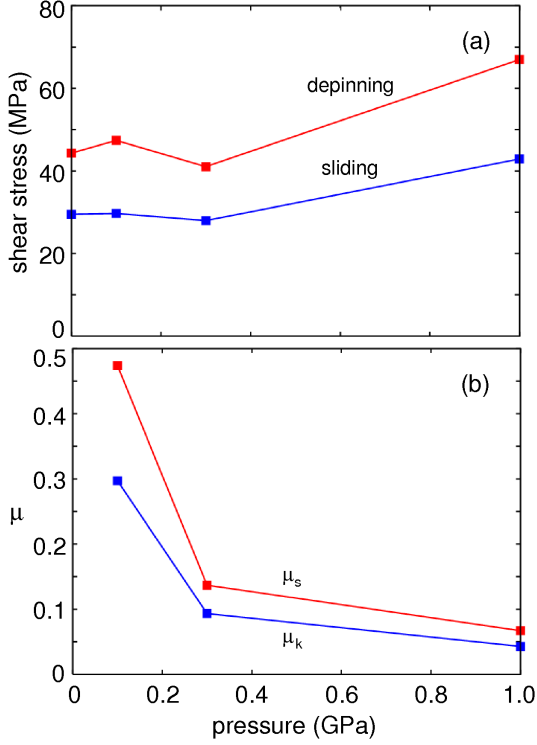


FIG. 9: The shear stress at depinning (static friction) and during sliding (kinetic friction) (a) and the static and kinetic friction coefficients (b) as a function of the applied pressure, for an elastic block sliding on a rough substrate. For the substrate with the root-mean-square roughness amplitude 3 Å. The elastic modulus of the block is $E = 10$ GPa.

$\sigma_c \alpha (F_N + F_{ad})$ so that the nominal frictional shear stress

$$\sigma_f = F_f / A_0 \approx \sigma_c \alpha (F_N + F_{ad}) / A_0 = \sigma_c \alpha (p + \sigma_a) \quad (3)$$

where $p = F_N / A_0$ is the (nominal) squeezing pressure and where the so called *detachment stress* [18, 20] σ_a gives a contribution to the frictional stress from the attractive wall-wall interaction. From (3) it also follows that the friction coefficient $\mu = \sigma_c \alpha (1 + \sigma_a / p)$ will diverge as the squeezing pressure p goes to zero.

We have studied the dependence of the frictional shear stress on the squeezing pressure for the system studied above, for the block elasticities $E = 10$ GPa and $E = 100$ GPa, and for the rigid substrate with the rms roughness amplitude 3 Å. In Fig. 9 we show (a) the (nominal) frictional shear stress and (b) the friction coefficient as a function of the squeezing pressure when $E = 10$ GPa. Note that, because of the attractive interaction, the frictional shear stress is constant for low squeezing pressures, while the friction coefficient diverges as $p \rightarrow 0$.

The adhesion contribution $\sigma_c \alpha \sigma_a$ to the frictional shear stress becomes important only when the elastic modulus of the block is small enough. The transition, with decreasing elastic modulus, from the case where the adhe-

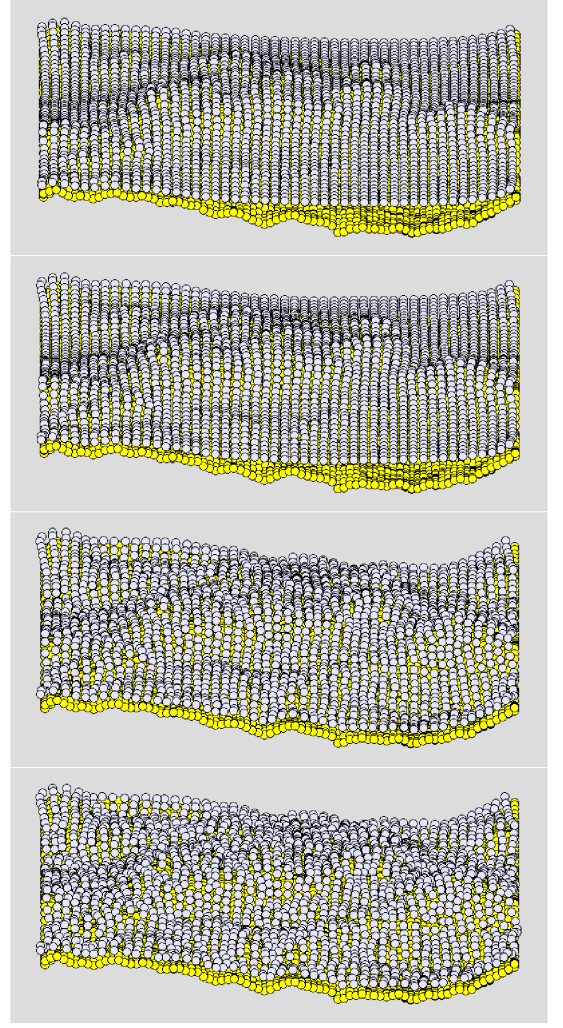


FIG. 10: The contact between an elastic block with a flat surface and a rough *rigid* substrate. Only the interfacial layers of atoms are shown. The elastic modulus of the block is $E = 1000, 100, 10$ and 5 GPa (from top to bottom). The substrate is self-affine fractal with root-mean-square roughness 3 Å. The applied pressure $p = 0.1E$. Note the elastic deformation of the block, and that the real contact area is smaller than the nominal contact area for high values of the elastic modulus of the block.

sion can be neglected to the case where it is important, is rather abrupt. To illustrate this we show in Fig. 10 the interfacial atoms (the top atoms of the substrate and the bottom atoms of the block) for blocks with the elastic modulus $E = 1000, 100, 10$ and 5 GPa, and with the squeezing pressure $p = 0.1E$. In the absence of adhesion all the systems would exhibit virtually identical arrangement of atoms. Indeed the two stiffest solids exhibit very similar atom-arrangements, but there is a clear change when E decreases from 100 to 10 GPa; in the latter case the attractive interaction is able to pull the solids into intimate contact over most of the nominal contact area. Thus the bottom surface of the block is able to bend and

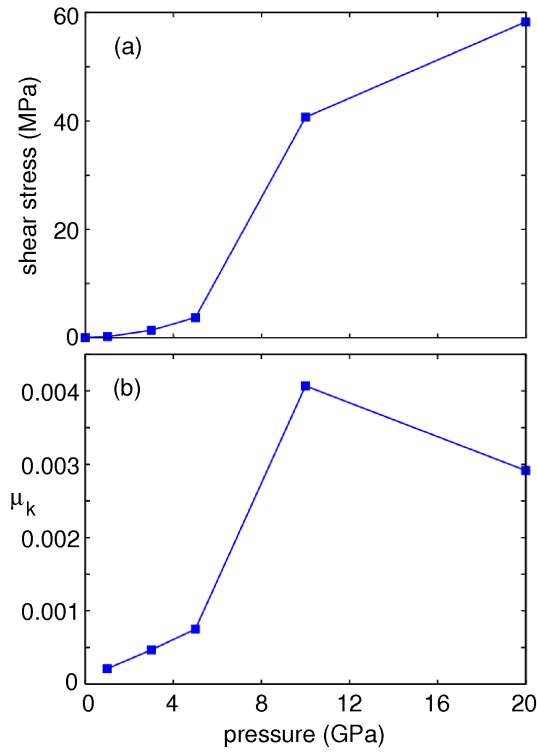


FIG. 11: The shear stress during sliding (kinetic friction) (a) and the kinetic friction coefficient (b) as a function of the applied pressure, for an elastic block sliding on a rough substrate. For the substrate with the root-mean-square roughness amplitude 3 Å. The elastic modulus of the block is $E = 100$ GPa.

fill out a substrate “cavity” with diameter D and height h if the gain in wall-wall binding energy, which is of the order of $D^2\Delta\gamma$ (where $\Delta\gamma$ is the interfacial binding energy per unit surface area for flat surfaces), is equal to (or larger than) the elastic energy stored in the deformation field in the block, which is of the order of $ED^3(h/D)^2$. This gives the “critical” elasticity $E_c \approx D\Delta\gamma/h^2$. In the present case we have a distribution of roughness wavelength but we can obtain a rough estimate of E_c by taking $h^2 = \langle h^2 \rangle = 9 \text{ Å}^2$ as the mean of the square of the roughness profile and $D \approx 100 \text{ Å}$ as a typical roughness wavelength. Using $\Delta\gamma \approx 4\epsilon/a^2 \approx 24 \text{ meV/Å}^2$ this gives $E_c \approx 40 \text{ GPa}$ which is between 100 and 10 GPa. This change in the contact mechanics has a large influence on the sliding friction. Thus, as we now will show, for the block with elastic modulus $E = 100 \text{ GPa}$ there will be a negligible contribution to the friction from the attractive interaction and $\sigma_a \approx 0$.

Fig. 11 shows the frictional shear stress for the same system as in Fig. 9 except that the elastic modulus of the block is ten times higher. In this case the influence of the attractive interaction is *negligible*, and the frictional shear stress decreases continuously as the squeezing pressure decreases. However, the friction coefficient

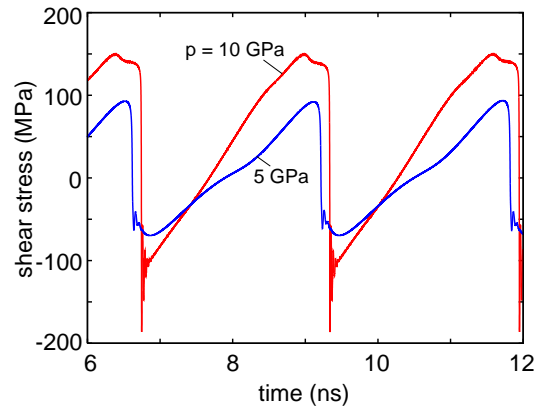


FIG. 12: The shear stress as a function of time for the rough substrate with the root-mean-square roughness amplitude 3 Å. The elastic modulus of the block is $E = 100 \text{ GPa}$ and the applied pressure $p = 5$ and 10 GPa .

is not constant as expected from the arguments presented above related to the invariance of the pressure distribution and contact size distribution with the squeezing force. This fact must be related to the small size of the system used in our simulations. As the squeezing pressure increases the stress distribution at the interface and the average size of the contact regions will change in such a way that when p increases from $p = 5$ to 10 GPa there is a very rapid increase in asperity contact regions undergoing elastic instabilities during sliding. This can be directly demonstrated by comparing the time-variation of the shear stress for $p = 5$ and 10 GPa , see Fig. 12. Note that at the higher pressure some slip events take place before the main slip event, i.e., new elastic instabilities appear and the frictional shear stress increases much faster than linear with the nominal squeezing pressure as p increases from 5 to 10 GPa .

To illustrate the small influence of the adhesion on the contact mechanics for the block with the elastic modulus $E = 100 \text{ GPa}$ we show in Fig. 13 the interfacial atoms for the squeezing pressures $p = 10, 3, 1 \text{ GPa}$ and 0 . When $p = 0$ only the adhesion pressure is acting and the area of real contact almost vanishes.

3.3. Role of adsorbates

Extremely low sliding friction is possible only in the absence of elastic instabilities. As shown above this is possible for stiff enough solids with incommensurate (or nearly incommensurate) surface structures. However, any types of imperfections may “lock” the surfaces together and introduce elastic instabilities during sliding. One type of “defect” discussed above is surface roughness. Another possibility is adsorbed molecules. Adsorbed molecules may arrange themselves at the interface between the two solids in such a way as to pin the solids together. A low concentration of (strongly bound) adsorbates is in many

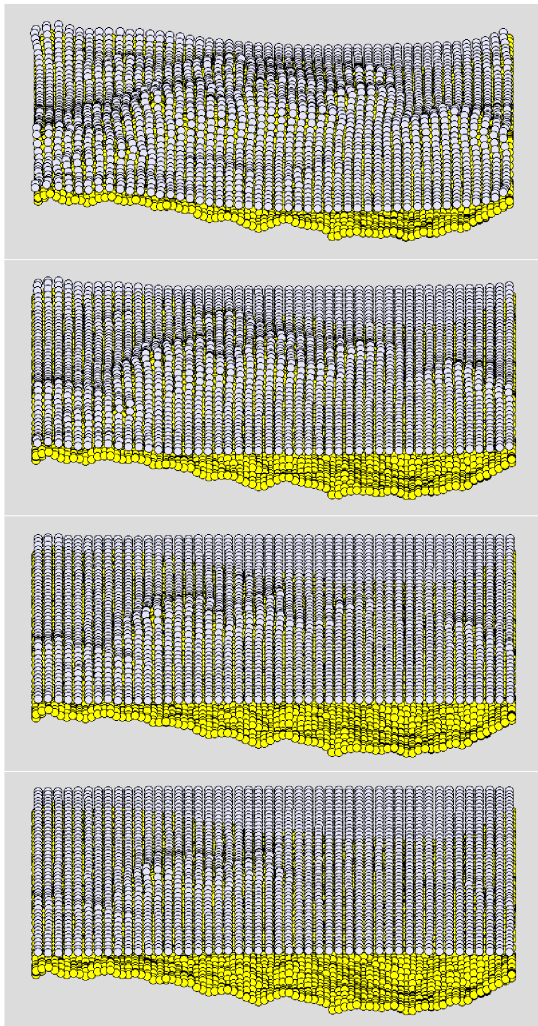


FIG. 13: The contact between an elastic block with a flat surface and a rough *rigid* substrate. Only the interfacial layers of atoms are shown. The elastic modulus of the block is $E = 100$ GPa. The substrate is self-affine fractal with root-mean-square roughness 3 \AA . The applied pressure $p = 10, 3, 1$ GPa and 0 (from top to bottom). For the latter case only the adhesion pressure is acting. Note the elastic deformation of the block, and that the real contact area is smaller than the nominal contact area.

ways similar to nanoscale roughness and it is clear that if the perfect system (flat surfaces without adsorbates) is in a superlubric state, one would expect a strong increase in the friction already at low adsorbate coverage. We have performed an extensive set of computer simulations to illustrate this effect both for atomically smooth surfaces and for rough surfaces. In Fig. 14 we show the kinetic friction coefficients for the elastic block ($E = 100$ GPa) sliding both on smooth and on rough substrates, as a function of liquid (octane, C_8H_{18}) coverage θ confined between two walls, for the applied pressure $p = 0.01E$ [21]. Note that for flat surfaces there is a very abrupt increase in the friction with increasing adsorbate cover-

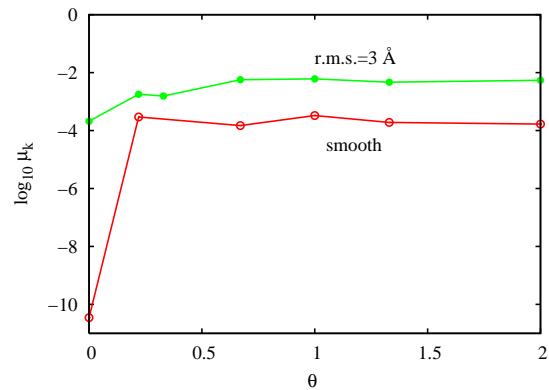


FIG. 14: The kinetic friction coefficients for the elastic block ($E = 100$ GPa) sliding both on smooth and on rough substrates, as a function of liquid coverage (octane, C_8H_{18}) θ confined between two walls [21]. The substrate has the root-mean-square (rms) roughness 3 \AA and the fractal dimension $D_f = 2.2$. The applied pressure $p = 1$ GPa.

age. In fact, the friction increases by a factor of $\sim 10^6$ as the coverage increases from zero to 0.22 monolayer. For $0.22 < \theta < 2$ the friction is nearly constant. For the rough surface the increase in the friction is much smaller. In this case the (small) increase in the friction results from octane molecules trapped in the asperity contact regions [22] – this results in an effectively increased surface roughness and enhanced friction.

4. Summary and conclusion

To summarize, we have studied the sliding of elastic solids in adhesive contact with flat and rough interfaces. We considered the dependence of the sliding friction on the elastic modulus of the solids. For elastically hard solids with planar surfaces with incommensurate surface structures we observe extremely low friction (superlubricity), which very abruptly increases as the elastic modulus decreases. Thus, at the superlubricity threshold, an increase in the elastic modulus by a factor of ~ 3 resulted in the decrease in the frictional shear stress by a factor $\sim 10^5$. We have shown that even a relatively small surface roughness, or a low concentration of adsorbates, may completely kill the superlubricity.

Acknowledgments

A part of the present work was carried out in frames of the ESF program “Nanotribology (NATRIBO)”. Two of the authors (U.T. and V.N.S.) acknowledge support from IFF, FZ-Jülich, hospitality and help of the staff during their research visits.

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- [1] B.N.J. Persson, *Sliding Friction: Physical Principles and Applications*, 2nd ed., Springer, Heidelberg, 2000.
- [2] S. Aubry, J. Phys. (Paris) **44**, 147 (1983).
- [3] B.N.J. Persson and E. Tosatti, Solid State Communications **109**, 739 (1999).
- [4] C. Caroli and P. Nozières, in *Physics of Sliding Friction*, ed. by B.N.J. Persson and E. Tosatti, Kluwer, Dordrecht (1996).
- [5] B.N.J. Persson, O. Albohr, F. Mancosu, V. Peveri, V.N. Samoilov and I.M. Sivebaek, Wear **254**, 835 (2003).
- [6] B.N.J. Persson, Phys. Rev. B **51**, 13568 (1995).
- [7] C. Caroli and P. Nozières, Eur. Phys. J. B **4**, 233 (1998).
- [8] T. Baumberger and C. Caroli, Advances in Physics **55**, 279 (2006).
- [9] K. Shinjo and M. Hirano, Surf. Sci. **283**, 473 (1993).
- [10] M.H. Müser, Europhys. Lett. **66**, 97 (2004).
- [11] E. Riedo and H. Brune, Applied Physics Letters **83**, 1986 (2003).
- [12] M. Dienwiebel, G.S. Verhoeven, N. Pradeep, J.W.M. Frenken, J.A. Heimberg and H.W. Zandbergen, Phys. Rev. Lett. **92**, 126101 (2004).
- [13] C. Yang, U. Tartaglino and B.N.J. Persson, Eur. Phys. J. E **19**, 47 (2006).
- [14] S. Hyun, L. Pei, J.F. Molinari, M.O. Robbins, Phys. Rev. E **70**, 026117 (2004).
- [15] B.N.J. Persson, O. Albohr, U. Tartaglino, A.I. Volokitin and E. Tosatti, J. Phys.: Condens. Matter **17**, R1 (2005).
- [16] B.N.J. Persson, J. Chem. Phys. **115**, 3840 (2001).
- [17] J.B. Sokoloff, Phys. Rev. E **73**, 016104 (2006).
- [18] B.N.J. Persson, Surface Science Reports **61**, 201 (2006).
- [19] B.V. Derjaguin, Wear **128**, 19 (1988); D. Tabor, in *Surface Physics of Materials*, Vol. II, edited by J.M. Blakely (Academic University Press, New York, 1975) p. 475.
- [20] B.N.J. Persson, Eur. Phys. J. E **8**, 385 (2002).
- [21] C. Yang, U. Tartaglino and B.N.J. Persson, J. Phys.: Condens. Matter **18**, 11521 (2006).
- [22] In the simulations the C_8H_{18} bed-units interact with the solid wall atoms via the Lennard-Jones potential with the well-depth parameter $\epsilon = 40$ meV. This relatively strong interaction leads to lubricant molecules trapped in the asperity contact regions. Other studies (see Ref. [21]) with $\epsilon = 5$ meV result in the squeeze-out of the lubricant from the asperity contact regions into the “valleys” or “cavities” of the substrate height profile. In this case, which we will report on elsewhere [21], we do not expect any adsorbate-induced increase in the friction.